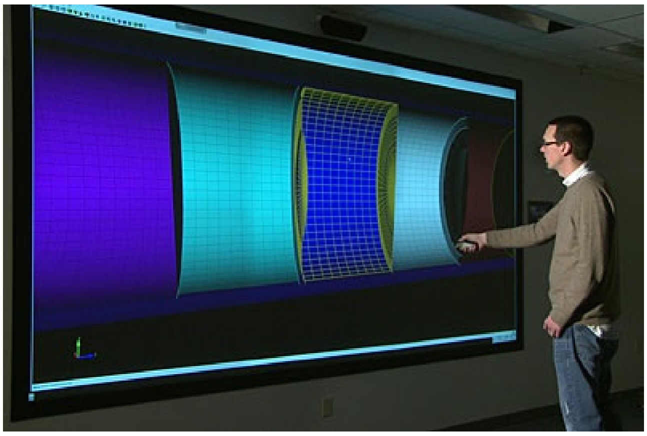


Predicting the behavior of complex systems — whether it's nuclear radiation impacts, heat/water flow in geothermal reservoirs or chemical migration through bedrock — is now easier thanks to the MOOSE simulation framework developed at INL.

INL's MOOSE drives nuclear materials, design innovation

By Nicole Stricker, *INL Communications & Governmental Affairs*

In nature, moose tend to be loners. But the one at Idaho National Laboratory is working with a bison, marmot, rat and others to make computer simulation more accessible and foster new collaboration opportunities.

The beast achieving all this is the Multiphysics Object-Oriented Simulation Environment, or MOOSE. This computer simulation framework advances the process for predicting the behavior of complex systems ranging from irradiation effects on materials to groundwater physics and chemistry.

INL's the MOOSE development team consists of, from left, David Andrs, John Peterson, Derek Gaston, Cody Permann and Jason Miller.

MOOSE makes it easier to create simulation capabilities for complex mathematical models, such as BISON, which has applications for nuclear reactor designers, or RAT, which simulates chemicals reacting and flowing through bedrock. It can even run two or more related models simultaneously to reveal new insights. Such simulations can help inform real-world experiments, and researchers no longer have to be computer science experts to tackle state-of-the-art simulation.

"People were doing these simulations before, but they had to develop the entire code," said Derek Gaston, the computational mathematician leading INL's Computational Frameworks Group. "Something that would take 5 years with a team of 10 people can now be done in 1 year with three people."

The power of modeling
Modeling and simulation have become indispensible research tools in nearly every branch of science. Mathematical models and computer simulations are particularly powerful for nuclear engineers studying irradiation's complex effect on materials and reactor components.

Such studies require expensive and time-consuming irradiation experiments. Researchers must fabricate test capsules, irradiate them for many months or years in a research reactor, let them cool after coming out of the reactor, and then do the post-irradiation examination. Most steps last 6 months or more, so it can take several years to get a single experimental result.

With modeling (i.e., a series of equations describing physical phenomena) and simulation (the solutions), every experiment has more impact — simulations can help focus experiments by suggesting when and why materials or components might fail under extreme irradiation.

"We can use modeling and simulation to design better experiments," said Steve Hayes, an INL nuclear engineer who leads irradiation testing and post-irradiation examination (PIE) for the U.S. Department of Energy's Fuel Cycle R&D program. "In the old days, you weren't sure what to try, so you'd do experiments with many variants and use PIE to see what worked and what didn't."

But now, engineers can build a mathematical model incorporating what they already know about radiation and material behavior, then use that model to perform a computer simulation that predicts outcomes under new conditions.

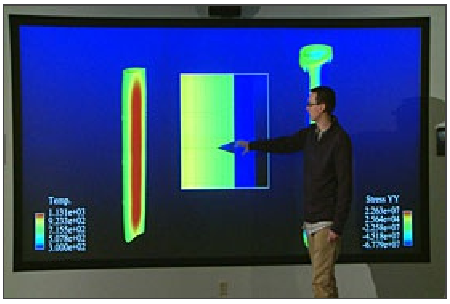
"Simulations can give a much better idea of what's going on, what will work and what won't," Hayes said. "So the experiment becomes a test to confirm what the model predicted."

MOOSE makes it easier
Building simulations is a time-consuming task requiring an entire team of people with detailed understanding of everything from parallel code development to the physics of the system under study. Most scientists are not programmers (and vice versa), so tackling simulation often proved too daunting.

But MOOSE carries much of the programming burden, making simulation tools more accessible for a wide array of researchers.

Although traditional simulation efforts tend to focus on one particular question, the MOOSE platform is a general problem solver that can accommodate many mathematical models. It essentially lets researchers "plug-and-play" by entering the mathematics describing their system — whether it's irradiation effects or groundwater movement — and letting MOOSE execute the simulation.

"Rather than spending all our effort to develop a simulation for one particular mathematical model, we put a lot of effort into the framework, which is then applicable to a range of models," said Gaston. "So we get more out of our effort and there's a bigger payoff."



Lead MOOSE developer Derek Gaston demonstrates some of its features in INL's Visualization Laboratory.

The seeds of that effort were planted roughly 7 years ago when Richard Martineau, director of INL's Fuels Modeling and Simulation Department, set out to bolster INL's high-performance computing capabilities. He started recruiting a multiphysics methods group, which now includes the MOOSE development team: Gaston, David Andrs, Cody Permann and John Peterson.

In 2008, they began developing the MOOSE framework by utilizing computer code and numerical libraries from existing, proven "massively scaling numerical tools" developed elsewhere in the DOE complex and academia. The result is a framework with a number of high-level features that impress their peers, including a "hybrid parallel mode" and "mesh adaptivity."

Plus, researchers don't have to access a supercomputer because MOOSE can also function at personal workstations. Best of all for scientists and engineers, it makes simulation capabilities more accessible to those who don't specialize in computational mathematics.

"The beauty of MOOSE is that it's a framework that takes care of that for you," Hayes said. "The user needs to know the governing equations for his or her field, and MOOSE solves them for you, meaning the scientist can focus on the science."

New pairings, increased teamwork
For Hayes, that focus is on the engineering-level components of new types of nuclear fuel, such as the metal cladding that encloses fuel pellets. Nuclear engineers like him want to know what makes cladding or other components fail under prolonged irradiation. Such phenomena can be informed by the work of materials scientists, who study radiation effects at the microscopic or atomic level.

MOOSE enables powerful simulations to be carried out without the use of a super computer.

Yet the two fields — microscopic and engineering-scale — have traditionally had little overlap. MOOSE is helping bring them closer by making it easy to merge their respective mathematical models into a single simulation.

BISON (BISON: Implicit Simulation Of Nuclear fuel) is the application that models nuclear fuel components on an engineering scale. Its microstructure equivalent is called MARMOT. MOOSE is able to run them both simultaneously to create a simulation that shows how radiation effects at the microscopic level evolve into fuel or cladding failures at the macroscopic level.

"BISON has produced an extremely high fidelity simulation of nuclear fuel rod behavior," Gaston said.

This sort of work has illustrated, for example, how tiny defects in nuclear fuel pellets can amplify over time to impact safety or energy production. This work helps the nuclear energy industry refine its understanding of operating margins to maximize efficiency without impacting safety.

In the future, MOOSE, BISON, MARMOT and a herd of associated programs can enable materials scientists to work hand-in-hand with nuclear engineers to achieve new insights far more quickly than was possible in the past.

"We hope to be able to mine every experiment for more useful data than ever before," Hayes said. "And we all hope this can reduce the number of experiments needed."

On the horizon
Nuclear engineers and materials scientists aren't the only ones benefiting from MOOSE. Geologists, geochemists and others have developed their own contributions to the modeling menagerie. RAT (ReActive Transport) is a program that can describe how more than a dozen different chemicals will interact as they flow through bedrock. And FALCON simulates water and heat flow in geothermal reservoirs.

Given the ease with which MOOSE can accommodate new models, more creatures are quickly joining the mix. Martineau, for one, is pleased that the framework has proven so useful for such a broad range of disciplines, though the impact for nuclear energy research is paramount.

"This work is helping the nuclear industry design safer and more efficient fuels," said Martineau. "Computational capabilities have always been important for nuclear materials research. But without the experiments, modeling and simulation is a useless exercise in mathematics and computation."

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